

Model Performance

Model	Data
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Weighted KNN model					
5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.87	0.81	0.87	0.82	0.86	0.86

Model Results

Predicted value: 3.29e-03 mol/L

Global applicability domain: Inside

Local applicability domain index: 6.19e-01

Confidence level: 3.63e-01

Nearest Neighbors from the Training Set

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Chloranil

Measured: 1.02e-03

Predicted: 3.29e-03

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2,5-Cyclohexadien-1-one, 2,6-dibromo-4-(chloroimino)-

Measured: 1.96e-04

Predicted: 1.41e-03

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Benzothiazole

Measured: 3.18e-02

Predicted: 2.15e-02

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Phthalazine

Measured: 3.84e-01

Predicted: 2.25e-02